Ward 10/670031

~ 07/28/2006

```
=> d his full
```

.- ---

```
(FILE 'HOME' ENTERED AT 14:24:44 ON 28 JUL 2006)
```

FILE 'REGISTRY' ENTERED AT 14:24:49 ON 28 JUL 2006 1.1 886180 SEA ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1 AND (>1 Q/REL))

L2 672553 SEA ABB=ON PLU=ON L1 AND NRRS>1

STRUCTURE UPLOADED L3

1 SEA SUB=L1 SSS SAM L3

D SCA

174 SEA SUB=L1 SSS FUL L3 L5 SAVE TEMP L5 WAR031STRA/A

FILE 'HCAPLUS' ENTERED AT 14:36:26 ON 28 JUL 2006 58 SEA ABB=ON PLU=ON L5 L6

FILE 'REGISTRY' ENTERED AT 14:36:35 ON 28 JUL 2006

FILE 'STNGUIDE' ENTERED AT 14:39:26 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 14:41:00 ON 28 JUL 2006

L7 STRUCTURE UPLOADED

7 SEA SUB=L5 SSS SAM L7 L8

D SCA

106 SEA SUB=L5 SSS FUL L7 L9

68 SEA ABB=ON PLU=ON L5 NOT L9 L10

FILE 'HCAPLUS' ENTERED AT 14:44:53 ON 28 JUL 2006 8 SEA ABB=ON PLU=ON L10 L11

FILE 'REGISTRY' ENTERED AT 14:45:01 ON 28 JUL 2006 SAVE TEMP L9 WAR031STRNT1/A

FILE 'STNGUIDE' ENTERED AT 14:53:21 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 14:58:12 ON 28 JUL 2006

L12STRUCTURE UPLOADED

L13 O SEA SUB=L5 SSS SAM L12

L143 SEA SUB=L5 SSS FUL L12 SAVE TEMP WAR031STRB/A L14

D SCA

FILE 'HCAPLUS' ENTERED AT 14:59:46 ON 28 JUL 2006 L15 1 SEA ABB=ON PLU=ON L14

FILE 'BEILSTEIN' ENTERED AT 15:00:01 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:00:12 ON 28 JUL 2006

L16 1 SEA ABB=ON PLU=ON L15 AND L11

60 SEA ABB=ON PLU=ON BULLINGTON J?/AU L17

3556 SEA ABB=ON PLU=ON FAN X?/AU L18

1783 SEA ABB=ON PLU=ON JACKSON P?/AU L19

47109 SEA ABB=ON PLU=ON ZHANG Y?/AU L20

3 SEA ABB=ON PLU=ON L17 AND (L18 OR L19 OR L20) L21

138 SEA ABB=ON PLU=ON L18 AND (L19 OR L20)
4 SEA ABB=ON PLU=ON L19 AND L20
138 SEA ABB=ON PLU=ON L18 AND L20
2 SEA ABB=ON PLU=ON L18 AND L19 L22

L23

L24

L25

2 SEA ABB=ON PLU=ON L24 AND (L17 OR L19) L26

```
FILE 'BEILSTEIN' ENTERED AT 15:03:41 ON 28 JUL 2006
```

FILE 'HCAPLUS' ENTERED AT 15:03:46 ON 28 JUL 2006

L27 6 SEA ABB=ON PLU=ON (L21 OR L23 OR L25 OR L26)

L28 1 SEA ABB=ON PLU=ON L27 AND (L16 OR L11)

D SCA

FILE 'BEILSTEIN' ENTERED AT 15:04:52 ON 28 JUL 2006

L29 0 SEA SSS SAM L3

L30 0 SEA ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1)

L31 0 SEA SSS SAM L12

L32 0 SEA SSS FUL L12

FILE 'MARPAT' ENTERED AT 15:07:07 ON 28 JUL 2006

L33 0 SEA SSS SAM L12

L34 1 SEA SSS FUL L12

D SCA

FILE 'REGISTRY' ENTERED AT 15:08:33 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:08:36 ON 28 JUL 2006

FILE 'STNGUIDE' ENTERED AT 15:08:47 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 15:08:57 ON 28 JUL 2006

D STAT QUE L5

D STAT QUE L9

D STAT QUE L14

FILE 'HCAPLUS' ENTERED AT 15:09:55 ON 28 JUL 2006

D QUE NOS L21

D QUE NOS L23

D QUE NOS L25

D QUE NOS L26 D QUE NOS L28

L35 6 SEA ABB=ON PLU=ON L21 OR L23 OR L25 OR L26 OR L28

FILE 'MEDLINE, EMBASE, BIOSIS' ENTERED AT 15:12:13 ON 28 JUL 2006

FILE 'STNGUIDE' ENTERED AT 15:12:17 ON 28 JUL 2006

FILE 'MEDLINE' ENTERED AT 15:12:34 ON 28 JUL 2006

L36 4 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

FILE 'EMBASE' ENTERED AT 15:13:54 ON 28 JUL 2006

L37 3 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

FILE 'BIOSIS' ENTERED AT 15:14:06 ON 28 JUL 2006

L38 3 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

FILE 'WPIX' ENTERED AT 15:14:24 ON 28 JUL 2006

L39 1 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

L40 0 SEA SSS SAM L3

L41 0 SEA SSS SAM L12

L42 2 SEA SSS FUL L12

SEL SDCN EDIT E1-E2 /SDCN /DCN

...

L43 1 SEA ABB=ON PLU=ON (RADZT1/DCN OR RADZT3/DCN)

SEL DCSE L42

EDIT E3-E4 /DCSE /DCRE

1 SEA ABB=ON PLU=ON (888697-0-0-0/DCRE OR 888700-0-0-0/DCRE) T.44

1 SEA ABB=ON PLU=ON L42/DCR L45

1 SEA ABB=ON PLU=ON (L43 OR L44 OR L45) L46

1 SEA ABB=ON PLU=ON L39 AND L46 L47

FILE 'STNGUIDE' ENTERED AT 15:18:30 ON 28 JUL 2006

FILE 'MEDLINE' ENTERED AT 15:19:08 ON 28 JUL 2006 D QUE L36

FILE 'EMBASE' ENTERED AT 15:19:22 ON 28 JUL 2006 D OUE L37

FILE 'BIOSIS' ENTERED AT 15:19:34 ON 28 JUL 2006 D QUE L38

FILE 'WPIX' ENTERED AT 15:19:47 ON 28 JUL 2006

D QUE L39

D QUE L47

1 SEA ABB=ON PLU=ON L39 OR L47 L48

FILE 'STNGUIDE' ENTERED AT 15:20:50 ON 28 JUL 2006

FILE 'HCAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 15:21:15 ON 28

JUL 2006

L49

L50

6 DUP REM L35 L36 L37 L38 L48 (11 DUPLICATES REMOVED) ANSWERS '1-6' FROM FILE HCAPLUS

D IBIB ABS HITSTR L49 1-6

FILE 'STNGUIDE' ENTERED AT 15:22:05 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 15:22:17 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:22:51 ON 28 JUL 2006 D STAT QUE L16

FILE 'BEILSTEIN' ENTERED AT 15:23:08 ON 28 JUL 2006 D STAT QUE L32

FILE 'MARPAT' ENTERED AT 15:23:32 ON 28 JUL 2006 D STAT QUE L34

FILE 'WPIX' ENTERED AT 15:23:45 ON 28 JUL 2006 D STAT QUE L46

FILE 'HCAPLUS, MARPAT, WPIX' ENTERED AT 15:24:48 ON 28 JUL 2006

1 DUP REM L16 L32 L34 L46 (2 DUPLICATES REMOVED)

ANSWER '1' FROM FILE HCAPLUS

D IBIB ABS HITSTR L50 1

FILE 'STNGUIDE' ENTERED AT 15:25:22 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:25:35 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 15:25:46 ON 28 JUL 2006

D STAT QUE L11 65 SEA ABB=ON PLU=ON L11 NOT L16

7 1

FILE 'STNGUIDE' ENTERED AT 15:26:45 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:26:59 ON 28 JUL 2006
7 SEA ABB=ON PLU=ON L11 NOT L16
D IBIB ABS HITSTR L52 1-7

FILE HOME

: .

L51

L52

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9 DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE HCAPLUS

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6 FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jul 21, 2006 (20060721/UP).

FILE BEILSTEIN

FILE LAST UPDATED ON JUNE 16, 2006

FILE COVERS 1771 TO 2006.

FILE CONTAINS 9,606,495 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

- * PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.
- * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE
- * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE
- * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.
- * FOR PRICE INFORMATION SEE HELP COST

*************** NEW

- * PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
- * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

FILE MARPAT

FILE CONTENT: 1961-PRESENT VOL 144 ISS 26 (20060721/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 2006118302 08 JUN 2006 DE 102004054303 11 MAY 2006 EP 1657292 17 MAY 2006 JP 2006120460 11 MAY 2006 WO 2006053912 26 MAY 2006 2419594 03 MAY 2006 GB FR 2877567 12 MAY 2006 RU 2275374 27 APR 2006 CA 2518664 10 MAR 2006

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

FILE MEDLINE

FILE LAST UPDATED: 27 Jul 2006 (20060727/UP). FILE COVERS 1950 TO DATE.

On December 11, 2005, the 2006 MeSH terms were loaded.

The MEDLINE reload for 2006 is now (26 Feb.) available. For details

. . . .

on the 2006 reload, enter HELP RLOAD at an arrow prompt (=>). See also:

http://www.nlm.nih.gov/mesh/

http://www.nlm.nih.gov/pubs/techbull/nd04/nd04 mesh.html

http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_med data changes.html

http://www.nlm.nih.gov/pubs/techbull/nd05/nd05 2006 MeSH.html

OLDMEDLINE is covered back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2006 vocabulary.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE EMBASE

FILE COVERS 1974 TO 28 Jul 2006 (20060728/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BIOSIS

FILE COVERS 1969 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 26 July 2006 (20060726/ED)

FILE WPIX

FILE LAST UPDATED:

24 JUL 2006

<20060724/UP>

MOST RECENT DERWENT UPDATE:

200647

<200647/DW>

DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE, PLEASE VISIT:

http://www.stn-international.de/training center/patents/stn guide.pdf <

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://scientific.thomson.com/support/patents/coverage/latestupdates/

>>> PLEASE BE AWARE OF THE NEW IPC REFORM IN 2006, SEE http://www.stn-international.de/stndatabases/details/ipc_reform.html and http://scientific.thomson.com/media/scpdf/ipcrdwpi.pdf <<<

>>> FOR FURTHER DETAILS ON THE FORTHCOMING DERWENT WORLD PATENTS INDEX ENHANCEMENTS PLEASE VISIT:

http://www.stn-international.de/stndatabases/details/dwpi r.html <<<

=>

=> file registry

4

FILE 'REGISTRY' ENTERED AT 15:08:57 ON 28 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9 DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d stat que L5

886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1 L1 AND (>1 Q/REL))

STR T.3

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3 STRUCTURE

100.0% PROCESSED 886160 ITERATIONS SEARCH TIME: 00.00.15

174 ANSWERS

QUERY(S)

=> d stat que L9

886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1 L1 AND (>1 Q/REL))

L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3 L5

1.7 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. "NOT" structure L9106 SEA FILE=REGISTRY SUB=L5 SSS FUL L7

100.0% PROCESSED 174 ITERATIONS SEARCH TIME: 00.00.02

106 ANSWERS

=> d stat que L14

L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1

AND (>1 Q/REL))

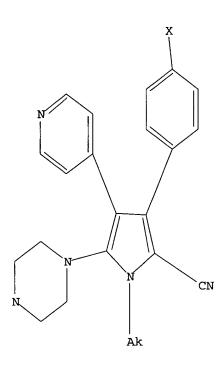
L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L5 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3

L12 STR



Structure attributes must be viewed using STN Express query preparation.

L14 3 SEA FILE=REGISTRY SUB=L5 SSS FUL L12

narrow structure

100.0% PROCESSED

9 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

=> file hcaplus FILE 'HCAPLUS' ENTERED AT 15:09:55 ON 28 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

AUTHOR SEARCH

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6 FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

d

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

```
=> d que nos L21
            60 SEA FILE=HCAPLUS ABB=ON PLU=ON
                                                BULLINGTON J?/AU
L17
          3556 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                FAN X?/AU
L18
          1783 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                 JACKSON P?/AU
L19
         47109 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                ZHANG Y?/AU
L20
             3 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                L17 AND (L18 OR L19 OR L20)
L21
=> d que nos L23
                                         PLU=ON
                                                JACKSON P?/AU
          1783 SEA FILE=HCAPLUS ABB=ON
L19
          47109 SEA FILE=HCAPLUS ABB=ON
                                         PLU=ON
                                                ZHANG Y?/AU
L20
              4 SEA FILE=HCAPLUS ABB=ON
                                         PLU=ON
                                                L19 AND L20
L23
=> d que nos L25
          3556 SEA FILE=HCAPLUS ABB=ON PLU=ON FAN X?/AU
L18
           1783 SEA FILE=HCAPLUS ABB=ON PLU=ON
                                                JACKSON P?/AU
L19
              2 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON L18 AND L19
L25
=> d que nos L26
             60 SEA FILE=HCAPLUS ABB=ON PLU=ON BULLINGTON J?/AU
L17
           3556 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON FAN X?/AU
L18
           1783 SEA FILE=HCAPLUS ABB=ON
                                         PLU=ON
                                                JACKSON P?/AU
L19
          47109 SEA FILE=HCAPLUS ABB=ON
                                         PLU=ON
                                                ZHANG Y?/AU
L20
                                         PLU=ON
                                                L18 AND L20
L24
            138 SEA FILE=HCAPLUS ABB=ON
                                         PLU=ON
                                                L24 AND (L17 OR L19)
L26
              2 SEA FILE=HCAPLUS ABB=ON
=> d que nos L28
         886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1
                AND (>1 Q/REL))
L3
                STR
            174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3
L5
L7
                STR
L9
            106 SEA FILE=REGISTRY SUB=L5 SSS FUL L7
             68 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L9
L10
              8 SEA FILE=HCAPLUS ABB=ON PLU=ON L10
L11
                STR
L12
              3 SEA FILE=REGISTRY SUB=L5 SSS FUL L12
L14
              1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14
L15
             1 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                L15 AND L11
L16
                                                 BULLINGTON J?/AU
L17
             60 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
           3556 SEA FILE=HCAPLUS ABB=ON
                                         PLU=ON
                                                 FAN X?/AU
L18
           1783 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                 JACKSON P?/AU
L19
          47109 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                 ZHANG Y?/AU
L20
              3 SEA FILE=HCAPLUS ABB=ON PLU=ON L17 AND (L18 OR L19 OR L20)
L21
```

```
4 SEA FILE=HCAPLUS ABB=ON PLU=ON L19 AND L20
T<sub>2</sub>3
          138 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L20
L24
            2 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 AND L19
L25
            2 SEA FILE=HCAPLUS ABB=ON PLU=ON L24 AND (L17 OR L19)
L26
            6 SEA FILE=HCAPLUS ABB=ON PLU=ON (L21 OR L23 OR L25 OR L26)
L27
            1 SEA FILE=HCAPLUS ABB=ON PLU=ON L27 AND (L16 OR L11)
L28
```

=> s L21 or L23 or L25 or L26 or L28 6 L21 OR L23 OR L25 OR L26 OR L28 L35

=> => file medline

FILE 'MEDLINE' ENTERED AT 15:19:08 ON 28 JUL 2006

FILE LAST UPDATED: 27 Jul 2006 (20060727/UP). FILE COVERS 1950 TO DATE.

On December 11, 2005, the 2006 MeSH terms were loaded.

The MEDLINE reload for 2006 is now (26 Feb.) available. For details on the 2006 reload, enter HELP RLOAD at an arrow prompt (=>). See also:

```
http://www.nlm.nih.gov/mesh/
http://www.nlm.nih.gov/pubs/techbull/nd04/nd04 mesh.html
```

http://www.nlm.nih.gov/pubs/techbull/nd05/nd05 med data changes.html

http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_2006_MeSH.html

OLDMEDLINE is covered back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2006 vocabulary.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d	que L36		
L17	- 60	SEA FILE=HCAPLUS ABB=ON PLU=ON BULLINGTON J?/AU	ı
L18	3556	SEA FILE=HCAPLUS ABB=ON PLU=ON FAN X?/AU	
L19	1783	SEA FILE=HCAPLUS ABB=ON PLU=ON JACKSON P?/AU	
L20	47109	SEA FILE=HCAPLUS ABB=ON PLU=ON ZHANG Y?/AU	
L36	4	SEA FILE=MEDLINE ABB=ON PLU=ON (L17 AND (L18 OF	L19 OR L20))
		OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L2	0 AND (L17 OR
		L19))	

=> file embase

FILE 'EMBASE' ENTERED AT 15:19:22 ON 28 JUL 2006 Copyright (c) 2006 Elsevier B.V. All rights reserved.

FILE COVERS 1974 TO 28 Jul 2006 (20060728/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que L37

```
Ward 10/670031
            60 SEA FILE=HCAPLUS ABB=ON
                                      PLU=ON BULLINGTON J?/AU
L17
          3556 SEA FILE=HCAPLUS ABB=ON
                                      PLU=ON
                                             FAN X?/AU
L18
          1783 SEA FILE=HCAPLUS ABB=ON PLU=ON JACKSON P?/AU
L19
         47109 SEA FILE=HCAPLUS ABB=ON PLU=ON ZHANG Y?/AU
L20
             3 SEA FILE=EMBASE ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20))
L37
               OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR
               1.19))
=> file biosis
FILE 'BIOSIS' ENTERED AT 15:19:34 ON 28 JUL 2006
```

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FILE COVERS 1969 TO DATE. CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 26 July 2006 (20060726/ED)

```
=> d que L38
            60 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON BULLINGTON J?/AU
L17
          3556 SEA FILE=HCAPLUS ABB=ON
                                        PLU=ON
                                                FAN X?/AU
L18
          1783 SEA FILE=HCAPLUS ABB=ON PLU=ON JACKSON P?/AU
L19
         47109 SEA FILE=HCAPLUS ABB=ON PLU=ON ZHANG Y?/AU
L20
             3 SEA FILE-BIOSIS ABB-ON PLU-ON (L17 AND (L18 OR L19 OR L20))
L38
               OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR
               L19))
```

=> file wpix FILE 'WPIX' ENTERED AT 15:19:47 ON 28 JUL 2006 COPYRIGHT (C) 2006 THE THOMSON CORPORATION

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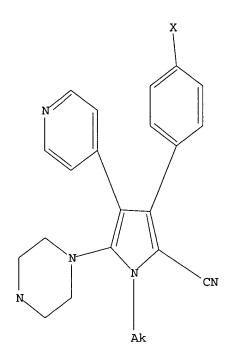
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http://www.stn-international.de/stndatabases/details/dwpi r.html <<< 'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

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PROCESSING COMPLETED FOR L38
PROCESSING COMPLETED FOR L48
              6 DUP REM L35 L36 L37 L38 L48 (11 DUPLICATES REMOVED)
L49
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L49 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:
                         2006:453871 HCAPLUS
TITLE:
                         Synthesis and SAR of \alpha-sulfonylcarboxylic acids
                         as potent matrix metalloproteinase inhibitors
                         Zhang, Yue-Mei; Fan, Xiaodong;
AUTHOR (S):
                         Xiang, Bangping; Chakravarty, Devraj; Scannevin,
                         Robert; Burke, Sharon; Karnachi, Prabha; Rhodes,
                         Kenneth; Jackson, Paul
                         Drug Discovery, Johnson & Johnson Pharmaceutical
CORPORATE SOURCE:
                         Research and Development, Raritan, NJ, 08869, USA
SOURCE:
                         Bioorganic & Medicinal Chemistry Letters (2006),
                         16(12), 3096-3100
                         CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER:
                         Elsevier B.V.
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     A series of novel carboxylic acid-based \alpha-sulfone MMP inhibitors
     have been synthesized and the in vitro enzyme SAR is discussed. A
     potential binding mode in the active site of the MMP-9 homol. model was
     highlighted. These compds. are potent MMP-9 inhibitors and are selective
     over MMP-1.
REFERENCE COUNT:
                         18
                               THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L49 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER:
                         2004:292020 HCAPLUS
DOCUMENT NUMBER:
                         140:321233
TITLE:
                         A preparation of pyrrole derivatives useful for the
                         treatment of disorders ameliorated by reduction of
                         TNF-\alpha production and/or p38 activity
INVENTOR (S):
                         Bullington, James L.; Fan, Xiaodong
```

; Jackson, Paul F.; Zhang, Yue-mei

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg. SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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20040408
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    WO 2004029040
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PRIORITY APPLN. INFO.:
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                                                                    20020927
                                            WO 2003-US30223
                                                                    20030924
OTHER SOURCE(S):
                       MARPAT 140:321233
GΙ
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 R^2 R^1 R^3 R^4 R^5 R^4 R^5 R^4 R^5 R^6 R^6 R^6 R^7 R^7

AB The invention relates to 3-pyridyl-4-arylpyrrole derivs. of formula I [wherein: R1 and R2 are independently selected from (un)substituted (hetero)aryl; R3 = H, (un)substituted alkyl, -N:CR6-, -C(O)R7, etc.; R4 = H, (un)substituted alkyl, (un)substituted (hetero)aryl, etc.; R5 =

(un) substituted alkyl, C(0)OR7, C(0)R7, CN, NO2, halo, etc.; R6 and R7 are independently selected from H, (un) substituted alkyl, (un) substituted aryl, (un) substituted heterocycle; with provisos], and pharmaceutical compns. comprising the same, useful for treating disorders ameliorated by reducing TNF- α production and/or p38 activity in appropriate cells. The invention compds. I were screened for p38 inhibition (in-vitro enzyme assays) and TNF- α inhibition (in-vitro whole cell assays and in vivo rodent assay). The invention also provides therapeutic and prophylactic methods using the instant pharmaceutical compns. For instance, pyrrole derivative II (compound 5; mouse 10 mg/kg, 0.5 h, 44% inhibition of TNF- α production) was prepared via condensation of 4-fluorobenzaldehyde with 4-pyridylacetonitrile, heterocyclization of the obtained pyridine derivative III with Me isocyanoacetate, N-methylation of the pyrrole ring of the obtained pyrrolecarboxylate derivative IV (X = H, R = H), bromination of the pyrrolecarboxylate derivative IV (X = H, R = Me), and subsequent amination of the obtained bromopyrrole derivative IV (X = Br, R = Me) by 4-(2-aminoethyl)morpholine.

IT 678161-35-8P 678161-52-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(intermediate; preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- α production and/or p38 activity)

RN 678161-35-8 HCAPLUS

CN

1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-52-9 HCAPLUS

CN 7-Indolizinecarboxylic acid, 1-(4-fluorophenyl)-5,6,7,8-tetrahydro-3-[[2-(4-morpholinyl)ethyl]amino]-8-oxo-2-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

IT 678161-34-7

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses) (preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF-α production and/or p38 activity)

RN 678161-34-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

IT 678161-38-1P 678161-40-5P 678161-41-6P 678161-42-7P 678161-54-1P 678162-27-1P 678162-29-3P 678162-34-0P 678162-35-1P 678162-36-2P 678162-37-3P 678162-39-5P 678162-41-9P 678162-43-1P 678162-45-3P 678162-46-4P 678162-47-5P 678162-50-0P 678162-51-1P 678162-52-2P 678162-53-3P 678162-61-3P 678162-62-4P 678162-69-1P 678162-70-4P 678162-71-5P 678162-72-6P 678162-73-7P 678162-75-9P 678162-93-1P 678162-99-7P 678163-05-8P 678163-25-2P

678163-26-3P 678163-28-5P 678163-29-6P 678163-30-9P 678163-33-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- α production and/or p38 activity)

RN 678161-38-1 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-40-5 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-[4-(methylsulfonyl)-1-piperazinyl]-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-41-6 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-[(ethylamino)carbonyl]-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-42-7 HCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(3-acetylphenyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-54-1 HCAPLUS CN 8(5H)-Indolizinone, 1-(4-fluorophenyl)-6,7-dihydro-3-[[2-(4-morpholinyl)ethyl]amino]-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

678162-27-1 HCAPLUS RN1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-CNmorpholinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

678162-29-3 HCAPLUS RN1H-Pyrrole-2-carboxylic acid, 1-methyl-3-(4-methylphenyl)-5-(1-CN piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 678162-34-0 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-N-propyl-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678162-35-1 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(1-methylethyl)-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678162-36-2 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(2-methylpropyl)-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678162-37-3 HCAPLUS

CN Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-

1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

Adding the second

RN 678162-39-5 HCAPLUS

CN Piperazine, 1-acetyl-4-[5-acetyl-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678162-41-9 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 678162-43-1 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

40 - 140,000

RN 678162-45-3 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-N,1-dimethyl-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678162-46-4 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(3,5-difluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 678162-47-5 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-N,N,1-trimethyl-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

,s)

RN 678162-50-0 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 678162-51-1 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(3-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 678162-52-2 HCAPLUS

CN Piperazine, 1-(cyclopropylcarbonyl)-4-[5-(cyclopropylcarbonyl)-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678162-53-3 HCAPLUS

CN 1H-Pyrrole-2-acetic acid, 3-(4-fluorophenyl)-1-methyl- α -oxo-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-61-3 HCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 5-(4

1H-Pyrrole-2-carboxylic acid, 5-(4-acetyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-62-4 HCAPLUS

CN Methanone, [3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]phenyl- (9CI) (CA INDEX NAME)

RN 678162-69-1 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-(4-ethyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

678162-70-4 HCAPLUS RN

1H-Pyrrole-2-carboxylic acid, 5-(4-cyclopentyl-1-piperazinyl)-3-(4-CNfluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

678162-71-5 HCAPLUS RN

1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-[4-(1-CN methylethyl)-1-piperazinyl]-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

678162-72-6 HCAPLUS RN

CN1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-propyl-1piperazinyl) -4 - (4 - pyridinyl) -, methyl ester (9CI) (CA INDEX NAME)

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RN 678162-73-7 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(cyclopropylmethyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

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RN 678162-75-9 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(cyclohexylmethyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-93-1 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-[(methoxymethylamino)carbonyl]-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 678162-99-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(hydroxymethyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 678163-05-8 HCAPLUS

CN Piperazine, 1-acetyl-4-[4-(4-fluorophenyl)-1-methyl-5-(1,3,4-oxadiazol-2-yl)-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678163-25-2 HCAPLUS

CN Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

12. 14.

678163-26-3 HCAPLUS RN

1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-CNmethyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)

678163-28-5 HCAPLUS RN

1-Piperazineacetic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-CNmethyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN

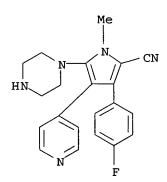
678163-29-6 HCAPLUS
Piperazine, 1-acetyl-4-[5-cyano-4-(4-fluorophenyl)-1-methyl-3-(4-CNpyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678163-30-9 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678163-33-2 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



L49 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2004:448213 HCAPLUS

DOCUMENT NUMBER: 140:404063

TITLE: Disruption of CCTβ2 expression leads to gonadal

dysfunction

AUTHOR(S): Jackowski, Suzanne; Rehg, Jerold E.; Zhang,

Yong-Mei; Wang, Jina; Miller, Karen;

Jackson, Pam; Karim, Mohammad A.

CORPORATE SOURCE:

Department of Infectious Diseases, St. Jude Children's

Research Hospital, Memphis, TN, 38105, USA

SOURCE:

Molecular and Cellular Biology (2004), 24(11),

4720-4733

CODEN: MCEBD4; ISSN: 0270-7306

PUBLISHER:

American Society for Microbiology

DOCUMENT TYPE:

Journal

LANGUAGE:

English

There are two mammalian genes that encode isoforms of CTP:phosphocholine cytidylyltransferase (CCT), a key rate-controlling step in membrane phospholipid biogenesis. Quant. determination of the CCT transcripts reveals

 $\mbox{CCT}\alpha$ is ubiquitously expressed and is found at the highest levels in the testis and lung, with lower levels in the liver and ovary. CCTB2 is a very minor isoform in most tissues but is significantly expressed in the brain, lung, and gonads. CCTB3 is the third isoform recently discovered in mice and is expressed in the same tissues as CCTB2, with its highest level in testes. We investigated the role(s) of CCT β 2 by generating knockout mice. The brains and lungs of mice lacking CCT β 2 expression did not exhibit any overt defects. On the other hand, a large percentage of the CCT β 2-/- females were sterile and their ovaries exhibited defective ovarian follicle development. proportion of female CCT β 2-/- mice with defective ovaries increased as the animals aged. The rare litters born from CCTβ2-/- + $CCT\beta 2-/0$ matings had the normal number of pups. The abnormal ovarian histopathol. was characterized by disorganization of the tissue in young adult mice and absence of follicles and ova in older mice, along with interstitial stromal cell hyperplasia which culminated in the emergence of tubulostromal ovarian tumors by 16 mo of age. Grossly defective CCTB2-/- ovaries were associated with high follicle-stimulating (FSH) and luteinizing (LH) hormone levels. Male CCTβ2-/0 mice exhibited progressive multi-focal testicular degeneration and reduced fertility but had normal FSH and LH levels. Thus, the most notable phenotype of CCT β 2 knockout mice was gonad degeneration and reproductive deficiency. The results indicate that although CCTB2 is expressed at very low levels compared to the α -isoform, loss of CCT β 2 expression causes a breakdown in the gonadal response to hormonal stimulation.

REFERENCE COUNT:

67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4

ACCESSION NUMBER:

2002:917652 HCAPLUS

DOCUMENT NUMBER:

138:137442

TITLE:

Regioselective Preparation of 2-Substituted 3,4-Diaryl

Pyrroles: A Concise Total Synthesis of Ningalin B

AUTHOR (S):

Bullington, James L.; Wolff, Russell R.;

Jackson, Paul F.

CORPORATE SOURCE:

Discovery Research, Johnson & Johnson Pharmaceutical Research and Development, L.L.C., Raritan, NJ, 08869,

USA

SOURCE:

Journal of Organic Chemistry (2002), 67(26), 9439-9442

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 138:137442

GI

المراجع المنتسر الأراجي المنتسر المنتسر

AB Me isocyanoacetate undergoes a 2 + 3 cycloaddn. with α,β -unsatd. nitriles to provide a regioselective synthesis of 2-substituted 3,4-diaryl pyrroles. The ease of preparation of α,β -unsatd. nitriles allows the rapid synthesis of pyrroles with varied substituents. Using this method, a key intermediate (I) for the synthesis of the marine natural products lukianol A, lamellarin O, and lamellarin Q was prepared in two steps. A total synthesis of ningalin B was also accomplished utilizing this methodol.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5

ACCESSION NUMBER: 2002:808686 HCAPLUS

DOCUMENT NUMBER: 138:205007

TITLE: Synthesis of pyrimido[4,5-b]indoles and

benzo[4,5]furo[2,3-d]pyrimidines via

palladium-catalyzed intramolecular arylation

AUTHOR(S): Zhang, Yue-Mei; Razler, Thomas;

Jackson, Paul F.

CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research and

Development, LLC, Raritan, NJ, 08869, USA

SOURCE: Tetrahedron Letters (2002), 43(46), 8235-8239

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:205007

GΙ

AB Various pyrimido [4,5-b] indoles and benzo [4,5] furo [2,3-d] pyrimidines were

synthesized via a palladium-catalyzed intramol. arylation of pyrimidine substrates. Thus, 4-aryloxy- or 4-anilino-5-iodopyrimidines, e.g. I, were treated with Pd(OAc)2(PPh3)2 and base in DMF to give the regioselective cyclized heterocycles, e.g. II.

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS 21 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6

ACCESSION NUMBER:

2002:607174 HCAPLUS

DOCUMENT NUMBER:

138:162771

TITLE:

Pyridinylimidazole based p38 MAP kinase inhibitors

AUTHOR (S):

Jackson, Paul F.; Bullington, James

CORPORATE SOURCE:

Discovery Research, Johnson and Johnson Pharmaceutical Research and Development, L.L.C., Raritan, NJ, 08869,

SOURCE:

Current Topics in Medicinal Chemistry (Hilversum,

Netherlands) (2002), 2(9), 1011-1020

CODEN: CTMCCL; ISSN: 1568-0266 Bentham Science Publishers Ltd.

PUBLISHER: DOCUMENT TYPE:

Journal; General Review

LANGUAGE:

English

45

A review. The p38 MAP kinase is thought to be involved in a variety of inflammatory and immunol. disorders such as rheumatoid arthritis. The pyridinylimidazole class of compds. was the first to potently inhibit this kinase. Since the original reports of their efficacy, they have become the most widely studied series of inhibitors of this kinase. This framework has served as a starting point for further synthetic work and several compds. have entered clin. trials. These compds. have also been utilized to elucidate the role of p38 kinase in the immune system, and more recently have been used to examine the role of this kinase in central nervous system disorders.

REFERENCE COUNT:

THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> file registry
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STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9 DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6 FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d stat que L16

L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1 AND (>1 Q/REL))

L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

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L7 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

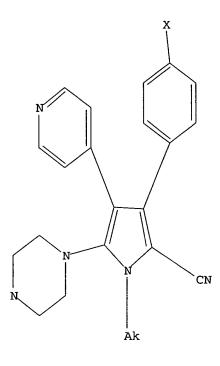
Structure attributes must be viewed using STN Express query preparation.

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L10 68 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L9

L11 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L10

L12 STR



Structure attributes must be viewed using STN Express query preparation.

L14 3 SEA FILE=REGISTRY SUB=L5 SSS FUL L12 L15 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14

L16 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 AND L11

=> file beilstein

FILE 'BEILSTEIN' ENTERED AT 15:23:08 ON 28 JUL 2006 COPYRIGHT (c) 2006 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON JUNE 16, 2006

FILE COVERS 1771 TO 2006.
*** FILE CONTAINS 9,606,495 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA

(reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

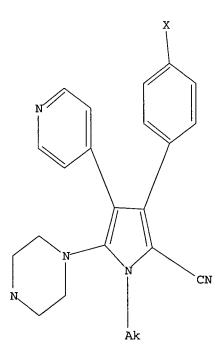
>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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NEW

- * PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
- * NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> d stat que L32 L12STR



Structure attributes must be viewed using STN Express query preparation. L32 O SEA FILE=BEILSTEIN SSS FUL L12

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.02

=> file marpat FILE 'MARPAT' ENTERED AT 15:23:32 ON 28 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

FILE CONTENT: 1961-PRESENT VOL 144 ISS 26 (20060721/ED)

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MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

2006118302 08 JUN 2006 DE 102004054303 11 MAY 2006 1657292 17 MAY 2006 EΡ 2006120460 11 MAY 2006 JΡ 2006053912 26 MAY 2006 WO 2419594 03 MAY 2006 GB 2877567 12 MAY 2006 FR 2275374 27 APR 2006 RU 2518664 10 MAR 2006 CA

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

=> d stat que L34 L12 STR

Structure attributes must be viewed using STN Express query preparation. 1 SEA FILE=MARPAT SSS FUL L12

100.0% PROCESSED 2804 ITERATIONS SEARCH TIME: 00.00.06

1 ANSWERS

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5444

FILE LAST UPDATED: 24 JUL 2006 <20060724/UP>
MOST RECENT DERWENT UPDATE: 200647 <200647/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:

http://www.stn-international.de/training_center/patents/stn_guide.pdf <

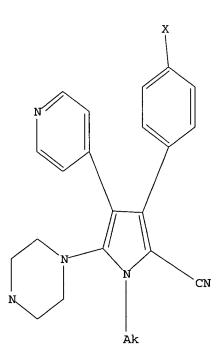
>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://scientific.thomson.com/support/patents/coverage/latestupdates/

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INDEX ENHANCEMENTS PLEASE VISIT:
http://www.stn-international.de/stndatabases/details/dwpi_r_html

http://www.stn-international.de/stndatabases/details/dwpi_r.html <<< 'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> d stat que L46 L12 STR



Structure attributes must be viewed using STN Express query preparation.

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1.45
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DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
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PROCESSING COMPLETED FOR L16
PROCESSING COMPLETED FOR L32
PROCESSING COMPLETED FOR L34
PROCESSING COMPLETED FOR L46
L50
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L50 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:
                            2004:292020 HCAPLUS
DOCUMENT NUMBER:
                            140:321233
                            A preparation of pyrrole derivatives useful for the
TITLE:
                            treatment of disorders ameliorated by reduction of
                            TNF-\alpha production and/or p38 activity
INVENTOR(S):
                            Bullington, James L.; Fan, Xiaodong; Jackson, Paul F.;
                            Zhang, Yue-mei
                            Janssen Pharmaceutica N.V., Belg.
PATENT ASSIGNEE(S):
                            PCT Int. Appl., 116 pp.
SOURCE:
                            CODEN: PIXXD2
DOCUMENT TYPE:
                            Patent
LANGUAGE:
                            English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                            KIND
                                    DATE
                                                APPLICATION NO. DATE
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                                               WO 2003-US30223
     WO 2004029040
                            A1
                                   20040408
                                                                            20030924
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         PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
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PRIORITY APPLN. INFO.:
                                              US 2002-414436P
                                                                      20020927
                                              WO 2003-US30223
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OTHER SOURCE(S):

MARPAT 140:321233

GI

NC

$$R^2$$
 R^1
 R^5
 R^4
 R^5
 R^6
 R^7
 R^8
 R^8

III

The invention relates to 3-pyridyl-4-arylpyrrole derivs. of formula I AB [wherein: R1 and R2 are independently selected from (un)substituted (hetero)aryl; R3 = H, (un)substituted alkyl, -N:CR6-, -C(O)R7, etc.; R4 = H, (un) substituted alkyl, (un) substituted (hetero) aryl, etc.; R5 = (un) substituted alkyl, C(O)OR7, C(O)R7, CN, NO2, halo, etc.; R6 and R7 are independently selected from H, (un) substituted alkyl, (un) substituted aryl, (un) substituted heterocycle; with provisos], and pharmaceutical compns. comprising the same, useful for treating disorders ameliorated by reducing TNF- α production and/or p38 activity in appropriate cells. The invention compds. I were screened for p38 inhibition (in-vitro enzyme assays) and $TNF-\alpha$ inhibition (in-vitro whole cell assays and in vivo rodent assay). The invention also provides therapeutic and prophylactic methods using the instant pharmaceutical compns. For instance, pyrrole derivative II (compound 5; mouse 10 mg/kg, 0.5 h, 44% inhibition of TNF- α

R

ΙV

production) was prepared via condensation of 4-fluorobenzaldehyde with 4-pyridylacetonitrile, heterocyclization of the obtained pyridine derivative III with Me isocyanoacetate, N-methylation of the pyrrole ring of the obtained pyrrolecarboxylate derivative IV (X = H, R = H), bromination of the pyrrolecarboxylate derivative IV (X = H, R = Me), and subsequent amination of the obtained bromopyrrole derivative IV (X = Br, R = Me) by 4-(2-aminoethyl)morpholine.

IT 678161-35-8P 678161-52-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(intermediate; preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- α production and/or p38 activity)

RN 678161-35-8 HCAPLUS

CN

1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-52-9 HCAPLUS

CN 7-Indolizinecarboxylic acid, 1-(4-fluorophenyl)-5,6,7,8-tetrahydro-3-[[2-(4-morpholinyl)ethyl]amino]-8-oxo-2-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

IT 678161-34-7

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses) (preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF-α production and/or p38 activity)

RN 678161-34-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 678161-38-1P 678161-40-5P 678161-41-6P
678161-42-7P 678161-54-1P 678162-27-1P
678162-29-3P 678162-34-0P 678162-35-1P
678162-36-2P 678162-37-3P 678162-39-5P
678162-41-9P 678162-43-1P 678162-45-3P
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678162-99-7P 678163-05-8P 678163-25-2P
678163-26-3P 678163-28-5P 678163-29-6P
678163-30-9P 678163-33-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use): BIOL (Biological study): PREP (Preparation): USES

75.

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of

(preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- α production and/or p38 activity)

RN 678161-38-1 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-40-5 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-[4-(methylsulfonyl)-1-piperazinyl]-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-41-6 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-[(ethylamino)carbonyl]-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-42-7 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(3-acetylphenyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678161-54-1 HCAPLUS 8(5H)-Indolizinone, 1-(4-fluorophenyl)-6,7-dihydro-3-[[2-(4-CN morpholinyl)ethyl]amino]-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

678162-27-1 HCAPLUS RNCN1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4morpholinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-29-3 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-3-(4-methylphenyl)-5-(1-piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 678162-34-0 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-N-propyl-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678162-35-1 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(1-methylethyl)-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678162-36-2 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(2-methylpropyl)-5-

(1-piperazinyl) -4-(4-pyridinyl) - (9CI) (CA INDEX NAME)

green, and the

RN 678162-37-3 HCAPLUS

CN Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-1+pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678162-39-5 HCAPLUS

CN Piperazine, 1-acetyl-4-[5-acetyl-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678162-41-9 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

678162-43-1 HCAPLUS RN

1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-CNpiperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

678162-45-3 HCAPLUS RN

1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-N,1-dimethyl-5-(1-CNpiperazinyl) -4 - (4 - pyridinyl) - (9CI) (CA INDEX NAME)

RN 678162-46-4 HCAPLUS

1H-Pyrrole-2-carboxylic acid, 3-(3,5-difluorophenyl)-1-methyl-5-(1-CN piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 678162-47-5 HCAPLUS

CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-N,N,1-trimethyl-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 678162-50-0 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

$$\mathbb{R}$$

PAGE 2-A

RN 678162-51-1 HCAPLUS
CN 1H-Pyrrole-2-carboxylic acid, 3-(3-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

مردوج مرا

RN 678162-52-2 HCAPLUS

CN Piperazine, 1-(cyclopropylcarbonyl)-4-[5-(cyclopropylcarbonyl)-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678162-53-3 HCAPLUS

CN 1H-Pyrrole-2-acetic acid, 3-(4-fluorophenyl)-1-methyl- α -oxo-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-61-3 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-(4-acetyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-62-4 HCAPLUS

CN Methanone, [3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]phenyl- (9CI) (CA INDEX NAME)

RN 678162-69-1 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-(4-ethyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-70-4 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-(4-cyclopentyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 678162-71-5 HCAPLUS

CN1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-[4-(1methylethyl)-1-piperazinyl]-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

678162-72-6 HCAPLUS RN

CN1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-propyl-1piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

678162-73-7 HCAPLUS RN

1H-Pyrrole-2-carboxylic acid, 5-[4-(cyclopropylmethyl)-1-piperazinyl]-3-(4-CN fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & Me \\ \hline MeO-C & N \\ \hline N & N \\ \hline \end{array}$$

RN 678162-75-9 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(cyclohexylmethyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & & \\$$

RN 678162-93-1 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-[(methoxymethylamino)carbonyl]-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 678162-99-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(hydroxymethyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

. :: ..

RN 678163-05-8 HCAPLUS

CN Piperazine, 1-acetyl-4-[4-(4-fluorophenyl)-1-methyl-5-(1,3,4-oxadiazol-2-yl)-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678163-25-2 HCAPLUS

CN Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678163-26-3 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 678163-28-5 HCAPLUS

CN 1-Piperazineacetic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\$$

RN 678163-29-6 HCAPLUS

CN Piperazine, 1-acetyl-4-[5-cyano-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

RN 678163-30-9 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

678163-33-2 HCAPLUS RNCN1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl) - (9CI) (CA INDEX NAME)

=> O

STRUCTURE SEARCH (BROAD)

=> file registry FILE 'REGISTRY' ENTERED AT 15:25:46 ON 28 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9 DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> file hcaplus FILE 'HCAPLUS' ENTERED AT 15:25:35 ON 28 JUL 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6 FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d stat que L11 L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1 AND (>1 Q/REL))

• •

STR

L3

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L5 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3

L7 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L9 106 SEA FILE=REGISTRY SUB=L5 SSS FUL L7

L10 68 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L9

L11 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L10

=> => s L11 not L16 L52 7 L11 NOT (L16)

- narrow structure search

=> d ibib abs hitstr L52 1-7

L52 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:559491 HCAPLUS

DOCUMENT NUMBER: 135:137517

TITLE: Preparation of pyridyl- and pyrimidinyl-substituted

fused pyrroles as cytokine inhibitors

INVENTOR(S): Striegel, Hans-Guenter; Laufer, Stefan; Tollmann

Neher, Karola; Tries, Susanne

PATENT ASSIGNEE(S): Merckle GmbH Chemisch Pharmazeutische Fabrik, Germany

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	TENT 1	. OV			KINI) :	DATE		i	APPL	ICAT:	ION I	NO.		D	ATE	
⇒ DE	1000	4157	-		A1		2001	0802		DE 2	000-3	10004	4157		20	0000	201
	2398							0809							20010131		
WO	2001	0570	12		A2		2001	0809	1	WO 2	001-1	EP10:	11		20010131		
WO	2001	0570	12		A3		2001	1227									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
								DZ,									
		HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,
		LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,
		SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	ŪĠ,	US,	UZ,	VN,
		YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM				
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		вJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG	•	•
EP	1252	163	•	-	A2	•	2002	1030	· ;	EP 2	001-	9023	70	•	2	0010	131
EP	1252	163			В1		2003	0924									
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR		•	•	,	•	•
JР	2003	5252:	27 [.]	•	T2	•	2003	0826	٠,	JP 2	001-	5578	73		2	0010	131
AΤ	2506	8 0			E		2003	1015		AT 2	001-	9023	70		2	0010	131
PT	1252							0227								0010	
ES	2208							0616								0010	131

NO 2002003634 Α 20020925 NO 2002-3634 20020731 US 2003153558 Α1 20030814 US 2002-182579 20021105 US 6867211 **B2** 20050315 20000201 PRIORITY APPLN. INFO.: DE 2000-10004157 Α 20010131 WO 2001-EP1011 W

OTHER SOURCE(S): GI

CASREACT 135:137517; MARPAT 135:137517

Title compds. [I; the first of R1-R3 = (substituted) 4-pyridyl, AΒ 2,4-pyrimidyl, 3-amino-2,4-pyrimidinyl; the second of R1-R3 = (substituted) Ph, thienyl; the third of R1-R3 = H, CO2H, alkoxycarbonyl, CH2OH, alkyl; R4, R5 = H, alkyl; X = CH2, S, O; n = 1, 2], and their use as pharmaceuticals is claimed. Thus, 3-(4-fluorophenyl)-2-(4-pyridyl)-5,6,7,8-tetrahydroindolizine-1-carboxylic acid Et ester (preparation given) in THF was treated dropwise at room temperature with NaAlH2(OCH2CH2OMe)2 in PhMe followed by stirring for 24 h at 40° to give 95% [3-(4-fluorophenyl)-2-(4-pyridyl)-5,6,7,8-tetrahydroindolizin-1yl]methanol. Several I inhibited tumor necrosis factor (TNFα), interleukin (IL-1β), 5-lipoxygenase, cyclooxygenase-1, and cyclooxygenase-2 with IC50 = 0.027-100 µmol.

351493-39-5P 351493-40-8P 351493-42-0P IT 351493-43-1P

Ι

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridyl- and pyrimidinyl-substituted fused pyrroles as cytokine inhibitors)

351493-39-5 HCAPLUS RN

1H-Pyrrolizine, 2,3-dihydro-5-methyl-7-phenyl-6-(4-pyrimidinyl)- (9CI) CN (CA INDEX NAME)

RN351493-40-8 HCAPLUS

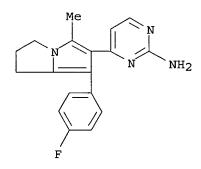
1H-Pyrrolizine, 7-(4-fluorophenyl)-2,3-dihydro-5-methyl-6-(4-pyrimidinyl)-CN (9CI) (CA INDEX NAME)

RN 351493-42-0 HCAPLUS

CN 2-Pyrimidinamine, 4-(2,3-dihydro-5-methyl-7-phenyl-1H-pyrrolizin-6-yl)-(9CI) (CA INDEX NAME)

RN 351493-43-1 HCAPLUS

CN 2-Pyrimidinamine, 4-[7-(4-fluorophenyl)-2,3-dihydro-5-methyl-1H-pyrrolizin-6-yl]- (9CI) (CA INDEX NAME)



L52 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:155517 HCAPLUS

DOCUMENT NUMBER: 124:202010

TITLE: Preparation of N-sulfonylpyrrolizineacetamides and

analogs as cyclooxygenase and lipoxygenase inhibitors

INVENTOR(S): Laufer, Stefan; Striegel, Hans Guenther; Dannhardt,

Gerd

PATENT ASSIGNEE(S): Merckle GmbH, Germany SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

			KIND DATE		APPLICATION NO.													
DE	4419	247			A1		1995	1207	Ι	DE 1	994-	4419	247		1:	9940	601	
CA	2191	746			AA		1995	1207		CA 1	995-	2191	746		1:	9950	531	
WO	9532	972			A1		1995	1207	V	VO 1	995-1	EP20	79		1	9950	531	
	W:	AM,	AU,	BB,	BG,	BR,	BY,	CA,	CN,	CZ,	EE,	FI,	GE,	ΗU,	IS,	JP,	KG,	
		ΚP,	KR,	KZ,	LK,	LR,	LT,	LV,	MD,	MG,	MN,	MX,	NO,	NZ,	PL,	RO,	RU,	
		SG,	SI,	SK,	ΤJ,	TT,	UA,	US,	UΖ,	VN								
	RW:	ΚE,	MW,	SD,	SZ,	UG,	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	
		LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,	MR,	NE,	
		SN,	TD,	TG														
AU	9526	730			A1		1995	1221	P	\U 1	995-:	2673	0		1:	9950	531	
EP	EP 763037			A1		1997	0319	E	EP 1	995-	9218	01		1	9950	531		
EP	7630																	
							ES,											SE
JP	1050	6370			T2		1998	0623	ن	JP 1	996-	5003	34		1:	9950	531	
JP	3671	303			B2		2005											
AT	2087	77			E	E 20011115			AT 1995-921801									
ES	2166	823			Т3					ES 1995-921801								
	7630													19950531				
	9605				Α		1996			VO 1	996-	5095			1:	9961	129	
	3100						2001											
	9604						1997			7I 1	996-	4773			1:	9961	129	
	1140						2004											
	5942				Α		1999											
PRIORIT	Y APP	LN.	INFO	.:									247					
		>								VO 1	995-1	EP20	79	Ţ	W 1:	9950	531	
OTHER SOURCE(S):			MAR	TAS	124:	2020	10											

$$R^7$$
 R^6
 R^2
 R^3

Ι

GI

_R5

R4

AB Title compds. [I; 2 of R1-R3 = H or (hetero)aryl and the other = COCO2H, alkoxycarbonyl, sulfonylcarbamoylalkyl, etc.; R4-R7 = H or alkyl; 2 vicinal R4-R7 = bond; X = CH2, O, S, (alkyl)imino, etc] were prepared Thus, title compound II had IC50 of 2.3x10-7 and 1.5x10-7 (units not given) against lipoxygenase and cyclooxygenase, resp.

IT 174348-04-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-sulfonylpyrrolizineacetamides and analogs as cyclooxygenase and lipoxygenase inhibitors)

RN 174348-04-0 HCAPLUS

CN Pyrrolo[2,1-b]thiazole-5-acetamide, 6-(5-chloro-2-thienyl)-2,3-dihydro-3-methyl-N-(methylsulfonyl)-7-phenyl- (9CI) (CA INDEX NAME)

L52 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:155516 HCAPLUS

DOCUMENT NUMBER: 124:202009

TITLE: Preparation of heteroarylpyrrolizineacetates and

analogs as cyclooxygenase and lipoxygenase inhibitors

; . .

INVENTOR (S): Laufer, Stefan; Striegel, Hans Guenther; Dannhardt,

Gerd

PATENT ASSIGNEE(S): Merckle GmbH, Germany

SOURCE: Ger. Offen., 25 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	PATENT NO.			DATE	APPLICATION NO.	DATE			
DE	£ 4419246		A1 19951207		DE 1994-4419246	19940601			
CA	2191747		AA	19951207	CA 1995-2191747	19950531			
WO	9532970		A1	19951207	WO 1995-EP2077	19950531			
	W: AM	, AU, BB,	BG, BR	, BY, CA,	CN, CZ, EE, FI, GE,	HU, IS, JP, KG,			
	KP.	, KR, KZ,	LK, LR	, LT, LV,	MD, MG, MN, MX, NO,	NZ, PL, RO, RU,			
	SG	, SI, SK,	TJ, TT	, UA, US,	UZ, VN				
	RW: KE	, MW, SD,	SZ, UG	, AT, BE,	CH, DE, DK, ES, FR,	GB, GR, IE, IT,			
	LU	, MC, NL,	PT, SE	, BF, BJ,	CF, CG, CI, CM, GA,	GN, ML, MR, NE,			
		, TD, TG							
AU	9526728				AU 1995-26728				
EP	P 763036		A1	19970319	EP 1995-921799	19950531			
EP	763036		B1	20020911					
	R: AT				GB, GR, IE, IT, LI,	LU, MC, NL, PT, SE			
JP	10506368	3	T2	19980623	JP 1996-500332	19950531			
-	3671302			20050713					
AT	223917		E		AT 1995-921799				
	763036		T		PT 1995-921799	19950531			
ES	2182903		T3	20030316	ES 1995-921799	19950531			
US	5958943		A	19990928					
NO	9605093		A	19961129	NO 1996-5093	19961129			
ИО	310291		B1	20010618					
FI	9604771		Α	19970127	FI 1996-4771	19961129			
FI	113964		B1	20040715					
PRIORITY	Y APPLN.	INFO.:			DE 1994-4419246	A 19940601			
					WO 1995-EP2077	W 19950531			
OMITTED OF	an /a/		*** ** ** **	124 2020	0.0				

OTHER SOURCE(S): MARPAT 124:202009

GI

Title compds. [I; 1 of R1-R3 = heteroaryl, 1 of the remaining = H or AB (hetero)aryl, and the remaining = H, CHO, carboxy(alkyl), alkoxycarbonyl, etc.; R4-R7 - H or alkyl; 2 of vicinal R4-R7 = bond; X = CH2, CO, O, S, etc.] were prepared Thus, title compound II had IC50 of 4x10-7 and 2x10-7 (units not given) against lipoxygenase and cycloxygenase, resp.

174348-04-0P IT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroarylpyrrolizineacetates and analogs as cyclooxygenase and lipoxygenase inhibitors)

174348-04-0 HCAPLUS RN

Pyrrolo[2,1-b]thiazole-5-acetamide, 6-(5-chloro-2-thienyl)-2,3-dihydro-3-CNmethyl-N-(methylsulfonyl)-7-phenyl- (9CI) (CA INDEX NAME)

L52 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1982:21285 HCAPLUS

DOCUMENT NUMBER: 96:21285

Lactone compounds containing an indolizine radical TITLE:

Becker, William J.; Farber, Sheldon; Hoover, Troy E. INVENTOR(S):

Appleton Papers, Inc., USA PATENT ASSIGNEE(S):

U.S., 15 pp. Cont.-in-part of U.S. 4,232,887. SOURCE:

CODEN: USXXAM

Patent DOCUMENT TYPE:

English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4275206	Α	19810623	US 1980-112500	19800116
US 4232887	Α	19801111	US 1979-17764	19790305
CA 1147728	A1	19830607	CA 1980-345510	19800212
SE 8001604	A	19800906	SE 1980-1604	19800229
SE 454696	В	19880524		
SE 454696	C	19880901		
FI 8000652	Α	19800906	FI 1980-652	19800303

FI 7	70035	В	19860131				
FI 7	70035	C	19860912				
BR 8	3001263	Α	19801104	BR	1980-1263		19800303
BE 8	382057	A1	19800904	BE	1980-199656		19800304
DK 8	3000913	A	19800906	DK	1980-913		19800304
NO 8	3000611	Α	19800908	NO	1980-611		19800304
ZA 8	3001238	Α	19810325	ZA	1980-1238		19800304
ES 4	189160	A1	19810401	ES	1980-489160		19800304
B TA	3001193	A	19840915	AT	1980-1193		19800304
AT 3	377761	В	19850425				
CH 6	556138	A	19860613	CH	1980-1714		19800304
NL 8	3001316	Α	19800909	NL	1980-1316		19800305
NL 1	174146	В	19831201				
NL 1	174146	C	19840501				
AU 8	3056161	A1	19800911	ΑU	1980-56161		19800305
AU 5	540061	B2	19841101				
DE 3	3008475	A1	19800918	DE	1980-3008475		19800305
	3008475	C2	19880526				
FR 2	2450858	A1	19801003	FR	1980-4999		19800305
	2450858	B1	19811016				
	2044284	Α	19801015	GB	1980-7564		19800305
	2044284	B2	19830420				
	55144054	A2	19801110	JP	1980-27848		19800305
	59044323	B4	19841029				
	1334072	Α	19820608		1980-192152		19800929
	3401458	A	19861215	AT	1984-1458		19840503
	383544	В	19870710				
PRIORITY	APPLN. INFO.:				1979-17764		19790305
					1980-112500	A	19800116
				ΑT	1980-1193	Α	19800304

OTHER SOURCE(S): MARPAT 96:21285

GI

Chromogenic compds. (I) for pressure- or heat-sensitive mark-forming record systems are prepared, where Z = pyridine-2,3-diyl, R = substituted or unsubstituted p-aminophenyl, indol-3-yl, or 1-carbethoxy-2-phenylindolizin-3-yl (Q), and R1 = Q. I give red to green colors when in contact with acidic substrates. Thus, condensation of 3-carboxy-1-pyridinyl-1-ethyl-2-methylindol-3-yl ketone [69898-42-6] with 1-carboethoxy-2-phenylindolizine [39203-59-3] in Ac2O gave crystalline II [76949-97-8], which produced a blue color when applied to a record sheet material coated with Zn-modified phenolic resin. Numerous other chromogenic compds. were similarly prepared

TT 76949-85-4P 76949-86-5P 76949-94-5P 76963-56-9P

RL: IMF (Industrial manufacture); PREP (Preparation)
 (preparation of, as color former for mark-forming record systems)
76949-85-4 HCAPLUS
Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

RN

CN

RN 76949-86-5 HCAPLUS
CN Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

RN 76949-94-5 HCAPLUS
CN Furo[3,4-b]quinoxalin-1(3H)-one, 3-(1-ethyl-2-methyl-1H-indol-3-yl)-3-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

RN 76963-56-9 HCAPLUS

CN Furo[3,4-b]pyrazin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

L52 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

1981:463688 HCAPLUS

DOCUMENT NUMBER:

95:63688

TITLE:

Chromogenic lactone compounds and their use in pressure-sensitive and thermosensitive recording

materials

INVENTOR(S):

Hoover, Troy Eugene; Farber, Sheldon; Becker, William

Joseph

PATENT ASSIGNEE(S):

Appleton Papers, Inc., USA

SOURCE:

GI

Ger. Offen., 98 pp. CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
DE 3008475	A1	19800918	DE 1980-3008475		19800305
DE 3008475	C2	19880526			
US 4232887	Α	19801111	US 1979-17764		19790305
US 4275206	Α	19810623	US 1980-112500		19800116
PRIORITY APPLN. INFO.:			US 1979-17764	Α	19790305
			US 1980-112500	Α	19800116

Chromogenic lactones containing an indolizinyl residue are prepared and used in pressure-sensitive recording materials, giving blue to green shades. Thus, a mixture of 1-ethyl-2-methylindol-3-yl 2-carboxyphenyl ketone [51389-84-5], 1-methyl-2-(2-naphthyl)indolizine [76949-58-1], and Ac20 was heated at 39° for 2 h to give I [76950-22-6], blue on a recording sheet coated with zinc-modified phenolic resin. Many similar lactones were prepared

TT 76949-85-4 76949-86-5 76949-94-5 76950-17-9 76963-56-9 77011-33-7

RL: USES (Uses)

(color formers, for copying paper, manufacture of)

Ι

RN 76949-85-4 HCAPLUS

CN Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

RN 76949-86-5 HCAPLUS

CN Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

RN 76949-94-5 HCAPLUS

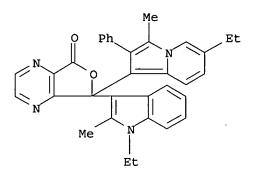
CN Furo[3,4-b]quinoxalin-1(3H)-one, 3-(1-ethyl-2-methyl-1H-indol-3-yl)-3-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

RN 76950-17-9 HCAPLUS

CN Furo[3,4-b]pyridin-7(5H)-one, 5-(1-ethyl-2-methyl-1H-indol-3-yl)-5-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

RN 76963-56-9 HCAPLUS

CN Furo[3,4-b]pyrazin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)



RN 77011-33-7 HCAPLUS

CN Furo[3,4-b]pyridin-7(5H)-one, 5-(1-ethyl-2-methyl-1H-indol-3-yl)-5-(6-ethyl-3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

L52 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

1981:425057 HCAPLUS

DOCUMENT NUMBER:

95:25057

TITLE:

Chromogenic lactone compounds and their use in pressure-sensitive and thermosensitive recording

materials

INVENTOR(S):

Hoover, Troy Eugene; Farber, Sheldon; Becker, William

Joseph

PATENT ASSIGNEE(S):

Appleton Papers, Inc., USA

SOURCE:

Ger. Offen., 67 pp.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3008494	A1	19800918	DE 1980-3008494	19800305
DE 3008494	C2	19890406		
US 4242513	Α	19801230	US 1979-17765	19790305
CA 1129855	A1	19820817	CA 1980-345054	19800205
SE 8001605	Α	19800906	SE 1980-1605	19800229
SE 454274	В	19880418		
SE 454274	С	19880728		
FI 8000653	Α	19800906	FI 1980-653	19800303
FI 69635	В	19851129		

FI	69635	C	19860310				
BR	8001247	Α	19801104	BR	1980-1247		19800303
BE	882056	A1	19800904	ΒE	1980-199655		19800304
DK	8000912	Α	19800906	DK	1980-912		19800304
NO	8000610	Α	19800908	ИО	1980-610		19800304
ZA	8001239	A	19810325	za	1980-1239		19800304
ES	489164	A1	19810401	ES	1980-489164		19800304
CH	656137	Α	19860613	CH	1980-1713		19800304
AT	8001192	Α	19880315	AT	1980-1192		19800304
AT	386833	В	19881025				
NL	8001317	Α	19800909	NL	1980-1317		19800305
NL	174737	В	19840301				
NL	174737	C	19840801				
AU	8056162	A1	19800911	ΑU	1980-56162		19800305
UA	539167	B2	19840913				
FR	2450857	A1	19801003	FR	1980-4934		19800305
FR	2450857	B1	19811030				
GB	2044285	Α	19801015	GB	1980-7565		19800305
GB	2044285	B2	19830420				
JP	55139455	A2	19801031	JP	1980-27847		19800305
JP	63020868	B4	19880430				
JP	58164642	A2	19830929	JP	1982-212045		19821202
JP	02048028	B4	19901023				
PRIORITY	Y APPLN. INFO.:			US	1979-17765	Α	19790305
				JΡ	1980-27847		19800305
a T							

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AB One hundred eleven chromogenic lactones I [R = H or RR = (CH:CH)2 (RR, R1 or R2 may be substituted); R1 = p-aminophenyl or benzimidazol-3-yl; R2 = a heterocyclic moiety comprised of 2 fused aromatic rings containing a N atom in

condensation-reactive position; X = X1 = CH or N, or X = N, X1 = CH] were prepared, which could be encapsulated to form pressure- and thermo-sensitive copying materials which could be activated by acidic clays or resins to provide uniform light-stable coloration. Thus, 1.23 g 6-(p-methoxyphenyl)imidazo[2,1-b]thiazole heated 3 h at 50-5° with 0.92 g 2-[(1-ethyl-2-methylindol-3-yl)carbonyl]benzoic acid in 30 mL Ac20 gave 2.1 g II, which provided, with acid clay, a purple recording material.

TT 76818-29-6P 76818-34-3P 76818-40-1P 76818-46-7P 76818-52-5P 76818-56-9P 76818-59-2P 76818-62-7P 76818-65-0P 76818-87-6P 76823-53-5P 76840-24-9P 76840-38-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and chromogenic property of)

RN 76818-29-6 HCAPLUS

1 (3H) -Isobenzofuranone, 3-[4-(diethylamino)-3-ethoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

RN 76818-34-3 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-[4-(diethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

RN 76818-40-1 HCAPLUS

CN 1(3H)-Isobenzofuranone, 4,5,6,7-tetrachloro-3-[4-(diethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

RN 76818-46-7 HCAPLUS

CN 1(3H)-Isobenzofuranone, 6-(dimethylamino)-3-[4-(dimethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

RN 76818-52-5 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)-3-[3-methoxy-4-[methyl(4-methylphenyl)amino]phenyl]-(9CI) (CA INDEX NAME)

RN 76818-56-9 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-[4-(cyclohexylamino)-3-methoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

RN 76818-59-2 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-[3-butoxy-4-(diethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

RN 76818-62-7 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)-3-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 76818-65-0 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-[4-(diethylamino)-3-methoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

RN 76818-87-6 HCAPLUS

CN Furo[3,4-b]pyridin-7(5H)-one, 5-[4-(diethylamino)-3-ethoxyphenyl]-5-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 76823-53-5 HCAPLUS

CN 1(3H)-Isobenzofuranone, 4,5,6,7-tetrachloro-3-[4-(diethylamino)-3-methoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

76840-24-9 HCAPLUS RN

CNFuro [3,4-b] pyridin-7 (5H) - one, 5-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo [1,2-methyl-2-phenyl-4H-pyrrolo [1,2-methyl-2-phenyl-4-phenyl-4-phenyl-4-phenyl-4H-pyrrolo [1,2-methyl-2-phenyl-4a]benzimidazol-3-yl)-5-(1,2,3,4-tetrahydro-1-methyl-6-quinolinyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 76840-38-5 HCAPLUS

CN Furo[3,4-b]quinolin-1(3H)-one, 3-[4-(diethylamino)-3-ethoxyphenyl]-3-(4ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA
INDEX NAME)

L52 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:89581 HCAPLUS

DOCUMENT NUMBER: 88:89581

TITLE: Hetarylation of indolizines

AUTHOR(S): Sheinkman, A. K.; Zherebchenko, V. I.; Stupnikova, T.

V.; Portsel, E.; Klyuev, N. A.

CORPORATE SOURCE: Dnepropetr. Inzh. Stroit. Inst., Dnepropetrovsk, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1977), (11),

1510-14

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 88:89581

GΙ

$$\mathbb{R}^2$$
 \mathbb{R}^2
 \mathbb{R}^1

AB Hetarylation of 2-methylindolizine I (R = R2 = H, R1 = Me) by quinoline and isoquinoline in the presence of BzCl gave in addition to I R = PhCO, R1 = Me, R2 = H), 60 and 33% I (R = 1-benzoyl-1,2-dihydro-2-quinolyl, 1-benzoyl-1,2-dihydro-2-isoquinolyl). Hetarylations with benzimidazole and imidazole in the presence of Ac2O gave 55% I (R = R2 = 1,3-diacetyl-4-imidazolin-2-yl, R1 = Me) and 93 and 30% I (R = R2 = 1,3-diacetylbenzimidazolin-2-yl, R1 = Me, Ph). Subsequent treatment of the imidazoline and benzimidazoline derivs. gave the corresponding

imidazolium and benzimidazolium perchlorates. Similar hetarylations were carried out with benzoxazole and acridine.

IT 65592-74-7P 65592-77-0P

RN 65592-74-7 HCAPLUS

CN 1H-Benzimidazole, 2,2'-(2-phenyl-1,3-indolizinediyl)bis[1,3-diacetyl-2,3-dihydro-(9CI) (CA INDEX NAME)

RN 65592-77-0 HCAPLUS

CN 1H-Benzimidazolium, 2,2'-(2-phenyl-1,3-indolizinediyl)bis[1,3-diacetyl-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 65592-76-9 CMF C36 H29 N5 O4

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM

CRN 14797-73-0 CMF Cl O4

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